

MIB Newsletter

Aug /Sept 2011

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More news and information about the MIB can be found on our website:

<http://www.mib.ac.uk/>

and in the [MIB brochure](#) available online



Research News

New academic in MIB – Clare Mills

We would like to welcome **Clare Mills** to the MIB community! Clare relocated from the BBSRC Institute for Food Research, Norwich, where she has been trying to unravel why food allergies occur and what foods cause them. Her appointment is in the Faculty of FMHS (School of Translational Medicine) and therefore strengthens our interactions with the Faculty. Her research interests in the molecular detail of allergic responses to food will strengthen our presence in the area of food security and map into the Biomolecular Mechanism and Catalysis theme of MIB. Clare will be giving a seminar in the near future to which we strongly encourage all to attend.

NaCTeM – assisting the creation of Clinical Trials.

A team from NaCTeM (housed within the MIB) has just completed work on a new TM system assisting the creation of clinical trials. The large amount of clinical trial data has led to an information overload problem, making it difficult to locate the precise information that is required. This project aims to address this problem through the development of a search application that can help users to narrow down their search efficiently, and assist in the creation of new protocols.



ASCOT (Assisting Search and Creation Of clinical Trials) is the search application being developed during this project. It applies text mining and data mining methods to large clinical trial collections, in order to enrich them with metadata. The different types of metadata added serve as effective tools for narrowing down searches. ASCOT additionally integrates a component for recommending eligibility criteria based on a set of selected protocols.

Search begins with a textual query. Then, it can be narrowed down in a multitude of ways:

- by selecting values for properties that correspond to XML fields of the clinical trial protocols.
- by selecting one of the automatically induced and labelled clusters of clinical trial protocols.
- by selecting a UMLS or SNOMED CT concept to occur in the (inclusion or exclusion) eligibility criteria of the clinical trial protocols.

- by selecting one of the multiword terms, automatically extracted by the C-Value algorithm.

The above alternatives can be applied iteratively until the result seems satisfactory to the user. The user can select documents and add them to a separate selection board for further processing. Probable eligibility criteria based on the selected documents are generated automatically.

Sophia Ananiadou Video and demonstrator are available here:
http://www.nactem.ac.uk/clinical_trials/

RNA Resonates at 1 GHz in the Dragon's World

Vasudevan Ramesh

I had the privilege of attending the 1st International Conference on the Chemical and Structural Biology of Nucleic acids and Proteins in Novel Drug Discovery on 12 – 14 June 2011 at Beijing in the Peoples Republic of China. The conference was held under the auspices of the Chinese Academy of Sciences and organised by the Peking University. The delegates included researchers from all over the world including well known scientific luminaries and two Nobel Laureates. The scientific programme was of a high standard touching on contemporary themes drawn from modern chemical and structural biology and was highly interdisciplinary in its content. As part of this programme, I delivered a lecture on the 1 GHz NMR of RNA – antibiotic interaction, thanks to the research work of the PhD students in my group which was well received.

As this was my first trip to China (Beijing), I was struck by the sheer enthusiasm and eagerness of the talented young Chinese research scholars hailing from various universities and institutes around the country. I have full admiration for these youngsters who were highly knowledgeable in their area of bioscience and fluent in communication. A highlight of the conference was an absorbing and brilliant plenary lecture given by Prof Yigong Shi at Tsinghua University on the “Mechanisms of Programmed Cell Death through Structural Biology” neatly delineating the various pathways which govern the initiation, execution and regulation of apoptosis. Prof Shi is a rising star and perhaps the readers might know that he was recently in the news for turning down an offer of Investigator of the Howard Hughes Medical Institute, U.S.A.

On the cultural delights, I had the exciting opportunity to climb the foot steps of the Great Wall (picture below) with the help of a tour guide. The accompanying saying written in Mandarin translates in English to *You are not a Man until you have climbed the Great Wall !!*



How I survived the HSE – a Pls perspective....

Roy Goodacre

When I was first told that the HSE is going to inspect my lab I immediately thought ‘Horrible

Scary Experience' and what a complete nightmare this may be! In fact, the actuality was rather different, and this visit was an almost pleasant experience, almost; but at the time, and the weeks running up to scrutinisation, I didn't know this...



As a PI, even though you know what's going on in your lab, and are aware that all the appropriate health and safety is in place, knowing you are going to be inspected and that every last detail will be under the microscope is not a pleasant feeling; microscope is a fairly apt term here as the HSE were particularly interested in our work on nanoparticles! The planning for one of these visits takes a lot of work, cooperation and preparation to feel half way comfortable about an official inspection from the HSE.

4 weeks to go...

- Initial meeting with MIB Safety Team, Chemistry Safety Team, University Health and Safety Services, and University compliance unit to discuss the visit and to begin preparations for it.
- Group meetings and emails to ensure all COSHH, risk assessments and chemical risk assessments are reviewed, correct and signed off.

3 weeks to go...

- More meetings with MIB Safety Team to discuss safety paperwork, review assessments and prepare for the inspection.
- Pre-inspection by MIB Safety Team and my lab manager to ensure housekeeping OK and no glaring hazards.
- Mock HSE inspection, involving group members, lab manager, University Safety Services, and MIB Safety Team.

1 week to go...

- Further lab meetings, emails, and meetings with MIB Safety Team to finalise all of the safety paperwork and ensure lab housekeeping is of high standard.

1 day to go...

- Final meeting with group members, lab manager and MIB Safety Team to discuss the upcoming inspection.
- Nice book to read at night to help with the inevitable insomnia...

Day of the inspection...

- Hearty breakfast (pause, not)
- MIB Safety Team met up with the HSE inspectors at University Safety Services for initial meeting
- Meeting with the inspectors in the MIB
- Inspection of lab areas and all relevant safety paperwork.
- Summing up meeting with HSE inspectors, who were very pleased with the standard of health and safety within the lab and the MIB as a whole.
- Later at home the 3Rs: Rest, Relaxation and a chat with my friend Ron...

As you can see - a lot of time, trouble and effort – but in the end a great result! I'd certainly like to pointed out that in addition to the excellent professional help from Tanya and the MIB Safety Team, to whom I am very grateful, I am also glad to have such a good research team who helped make sure the labs were up to snuff; the benches have never sparkled so much! In particular, much thanks goes to David Ellis (our lab manager who helped with the meticulous planning) and Lorna Ashton (who demonstrated our Raman facilities to the HSE). A very big thanks also goes to two PhD students Sam Mabbott and Dave Cowcher who demonstrated our nanoparticle H&S procedures to the HSE team; I was very pleased to be told afterwards by the HSE nanomaterials expert that he was very impressed with them; well

done chaps!

Safety first..!



If you have any health and safety concerns, please contact the Safety Office.

Email: tanya.aspinall@manchester.ac.uk
Phone: 306 5187 (internal: 65187)

Focus on...Safety Training

The table below shows details of the MIB H&S training courses to be held at the end of September for all new postgraduate students (which includes Masters, MChem, PhD students, etc).

All courses are **COMPULSORY** for all new postgrad students planning to work in the MIB labs – **failure to attend the complete course will result in the students not being permitted to work in the MIB labs.** Please let new students in your groups know about the courses.

All of the sessions are also open to everyone currently in the MIB, and are a good source of refresher H&S training.

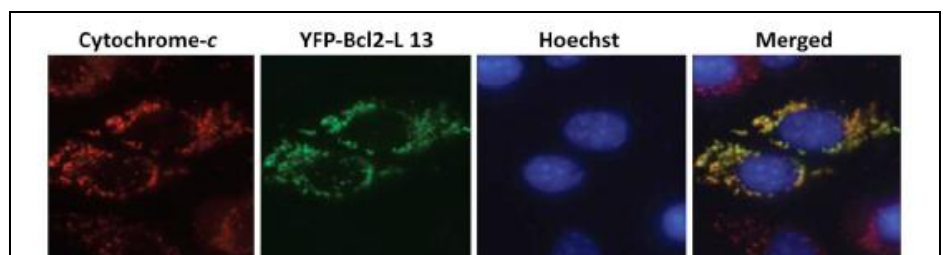
Date	Time	Course
28/09/11	2 – 3.30pm	MIB H&S induction
29/09/11	11.30 – 1pm	Working in the MIB labs, good lab practice and lab safety
	2 – 4pm	Risk assessment and COSHH assessment
30/09/11	10 – 12pm	Working with biological agents – awareness training (inc. safety cabinets)
	2 – 3.30pm	Chemical Safety – including specialised burns + cryogenics

Anne-Marie Buckle memorial prize

The memorial prize was set up last year by the Faculty of Life Sciences to commemorate Anne Marie Buckle's commitment and enthusiasm for both teaching and research. The award is awarded for the best final year student project in the general area of Cell and Molecular Biology. This year the award has been presented to **Christopher Gallagher** who for his project "*The novel Bcl-2 protein, Bcl2-Like 13, is a mitochondrial substrate of p38 Mitogen-Activated Protein Kinase (p38MAPK)*".

Christopher gained a 1st class degree in Pharmacology with Industrial Experience.

Scientific summary:



Most cells undergo apoptosis via the intrinsic pathway. A critical process in intrinsic apoptosis is mitochondrial outer membrane permeabilisation (MOMP), the point in which a cell has become dedicated to die. The Bcl-2 protein family are key regulators in the intrinsic apoptotic pathway with the activation of proapoptotic Bcl-2 proteins Bax and Bak ultimately responsible for mediating MOMP. What is less well understood is how Bax and Bak are activated on the outer mitochondrial membrane (OMM) to trigger cell death. We have previously identified that mitochondrial p38MAPK regulates Bax activation, but the p38MAPK substrates involved in this process remain to be determined. A proteomic screen has identified Bcl2-L 13 as a potential p38MAPK substrate and the aim of this project was to investigate further the relationship between Bcl2-L 13 and p38MAPK. Bcl2-L 13 is an uncharacterised Bcl-2 protein with reported pro-apoptotic and anti-apoptotic functions. In this report we generated and characterised a YFP-tagged Bcl2-L 13 expression construct. A phosphorylation assay was then performed by expressing YFP-Bcl-L 13 in DKO cells in combination with active or inactive mitochondrial p38MAPK. Immunoprecipitation of the YFP-Bcl2-L13 from the cell lysates allowed us to identify p38MAPK-dependent phosphorylation of Bcl2-L 13 via immunoblotting with phospho-specific MAPK substrate antibodies and also by mass spectrometry. We also identified a binding interaction between Bcl2-L 13 and p38MAPK as p38MAPK was present in our YFP-Bcl2-L 13 immunoprecipitation. Thus, in addition to confirming that Bcl2-L 13 is phosphorylated by p38MAPK, we suggest that Bcl2-L13 may be a novel p38MAPK scaffold protein acting to recruit p38MAPK to the outer mitochondrial membrane, where its activity ultimately results in Bax activation.

Funding News

MIB Promoting Interface Networking (PIN) initiative – Sept 2011

This initiative is intended to promote successful interface research. Deadline for applications: 11th October.

Primary objective: *to provide financial, personal and professional support to academics in MIB either to move research in new directions or form new collaborations.*

This round of funding could be for:

1. Projects that link research themes across MIB.
2. Collaborations with researchers external to MIB towards future grant funding.
3. Public engagement activities that promote MIB science/lead to further public engagement funding.
4. Younger researchers for career development (establishing collaborations, etc).
5. Travel and subsistence for PI's to foster an international collaboration towards future funding.

Alternative proposals will also be considered!

This funding should be targeted towards a concrete aim – e.g moving research in a new direction towards future grant funding.

What we can provide to successful applicants to the scheme: Financial awards of up to £5K per applicant – this could cover consumable costs, travel or subsistence, access to core facilities (across campus). The awards will be closely monitored by the research strategy group and advice and guidance provided when required.

Please contact [Ros](#) to submit applications or for further information.

NC3Rs research competition to link academia and industry

This year the NC3Rs is launching a new initiative called CRACK-IT. A key aim of CRACK-IT is to develop new technologies (products, models and tools) for industry which reduce reliance on animal research (the 3Rs). This will be achieved by connecting and funding

scientists from academia and industry. CRACK-IT will include a research competition designed to solve business challenges with a 3Rs theme identified with the pharmaceutical, chemical, agrochemicals and consumer product industries. This is an NC3Rs/industry partnership with the NC3Rs providing research funding and the companies sponsoring the challenges via in kind contributions including, data, equipment, samples and compounds. The research competition will be run through the TSB's Small Business Research Initiative. Further information can be found at www.nc3rs.org.uk/crackit

NSF/EPSC Chemistry Proposals 2011

Invitation for outlines: International Collaboration in Chemistry between US Investigators and their Counterparts in the UK (ICC).

Closing Date: 04-11-2011

<http://www.epsrc.ac.uk/funding/calls/open/Pages/nsfepsrcchemistry.aspx>

EPSC: Energy Storage Grand Challenge: Integrating Energy Storage for Future Energy Networks

Invitation for outlines: This challenge focuses on the electricity grid as we move towards 2050. The ambition of a Grand Challenge should be far greater than what can be achieved by a single research team or in the span of a single research grant.

Closing Date: 02-11-2011 [Website](#)

EPSC: Nanoscale technology Enabled healthcare: building the supply chain

Invitation for proposals: The Technology Strategy Board, in partnership with EPSC, is to invest up to £9m in grant funding to support highly innovative, business led collaborative research projects focussed on nanoscale technology-enabled solutions for the healthcare sector. Closing Date: 06-12-2011 [Website](#)

BBSRC-Brazil (FAPESP) joint funding of research

This award is run jointly with Brazil's São Paulo Research Foundation (FAPESP). See the guidance notes for more details.

Aim

- To pump-prime collaborations between scientists in the UK and the São Paulo State, Brazil
- To promote the exchange of scientists and access to facilities and materials
- To encourage applications under the RCUK-FAPESP lead agency agreement
- To enhance food security and bioenergy and industrial biotechnology research in the UK and Brazil

Scope

- Typically up to £35k over 2-years will be provided for the UK partners
- FAPESP will provide similar funding to Brazilian scientists
- Funds are mainly for networking and travel costs, but some modest research costs may be included (see guidance)
- Research groups should try and access other sources of funding in addition to the FAPESP
- Brazilian partners may wish to explore additional mutual funding

For further details see [website](#)

International Scientific Interchange Scheme (ISIS)

Application deadline: apply at any time*

***at least 6 weeks before travel**

Aim To help scientists add an international dimension to their BBSRC funded research by making and establishing new contacts with international counterparts

Scope: Funding is available for:



Congratulations to PhD student prize winners

Ross Chawner, a final year student under the supervision of Claire Evers in the Michael Barber Centre for Mass Spectrometry, was fittingly awarded the Barber Prize for the best oral presentation at the 32nd meeting of the British Mass Spectrometry Society (BMSS). Being the 30th Anniversary celebration of the development of Fast Atom Bombardment (FAB) by Michael Barber, it was particularly welcome to bring this award 'home'. In recognition, Ross received £250 prize money and will be chairing one of the sessions at the 33rd BMSS conference. Well done Ross!

Victoria Brewster – was awarded the Poster prize at the conference: 'Future technologies in downstream bioprocessing' in London on the 19th September. Her poster was called 'vibrational spectroscopy and chemometric modelling: applications in downstream bioprocessing'.

Recent Grant Awards

Ardeshir Bayat has been awarded approximately £77K by Glaxosmithkline Res & D for his work on "*Validation of inhibition of TGF β antibody 1D11*"

Robin Curtis (PI), Jim Warwicker, Alan Dickson and Jeremy Derrick have received funding from BBSRC for their 3yr project "Understanding and predicting aggregation in biopharmaceuticals" (Value £711K)

Roy Goodacre (Col), Tarani Chandola, Michael Horan, James Nazroo (PI), Neil Pendleton, Gindo Tampubolon, Frederick Wu and Alistair Burns have been awarded approx £1.7M from MRC for work on "Inequalities in later life frailty and wellbeing: an interdisciplinary approach to causality"

Hans Westerhoff (PI), Goodacre Royston and Alan Dickson have been awarded a BBSRC grant of approx £820K for work on "Predictable Protein Production".

Joshua Knowles (PI) and Roy Goodacre have received 1 yr funding from BBSRC "MUSCLE: Multi-platform Unbiased-optimisation of Spectrometry via Closed-Loop Experimentation" (£27K)

Roy Goodacre, Jean-Marc Schwartz, Caroline Bowsher and Giles Johnson (PI) have been awarded BBSRC funding for a project "Enhancing leaf transient carbon stores - role of fumarate as a possible storage compound"

Aline Miller (PI) and Roy Goodacre have received industrial funding from Solvay for research into "Peptide and Oligonucleotide Based Biomaterials" this funding (£1.4M) is with co-applicants from across the University with colleagues (Elena Bichenkova, Julie Gough, Leszek Majewski, Catherine Merry, Alberto Saiani, Michael Turner) from the School of Pharmacy and Pharmaceutical Sciences, Chemistry, Materials, Electrical and Electronic Engineering, and Chemical Engineering & Analytical Sciences.

John Keane and colleagues from the Manchester Business School (Nikolay Mehandjiev (PI) and Pedro Sampaio) have received EU funding (£143K) for the project "Building service testbeds on FIRE".

Nicholas Lockyer (PI), Adam McMahon (Wolfson Imaging centre) and Kaye Williams

(School of Pharmacy) have had their project "Quantitative Nanoscale Imaging of trace elements in biological systems" funded by the BBSRC (£150K)

Births

Congratulations to **Paul Mulherin** whose wife gave birth to a healthy baby boy (weighing 8lb 8oz) they have named him Christopher James Mulherin.

Diane Short (now in FLS accounts) has given birth to a little boy – Konnor – He weighed in at 7lb 8oz.

Seminars & Events

[TOP](#)

Seminars in MIB

MIB International seminar series

24th November - **Prof. Volker Deckert**, Jena University hosted by Roy Goodacre

MIB mini research conference - Wednesday 26th October 2011

The afternoon event, for ALL researchers and academics within MIB, will commence at 13.30 with a short open meeting hosted by the director of the MIB, Nigel Scrutton. The event will see a series of short talks from MIB postgraduate and postdoctoral researchers, together with short presentations from MIB academics and finish with a drinks reception to welcome our new PhD students to the MIB – all are expected to attend. Nominations for speakers are still welcome! (email [Ros](#))

[Faculty of Life Sciences](#) AZ Seminar series

Pharmacy <http://www.pharmacy.manchester.ac.uk/aboutus/events/seminars2010/>

School of Chemical Engineering and Analytical Science <http://www.ceas.manchester.ac.uk/research/seminar/>

School of Chemistry <http://www.chemistry.manchester.ac.uk/research/seminars/>

School of Computer Science <http://www.cs.manchester.ac.uk/research/seminars/school/>

School of Materials <http://www.materials.manchester.ac.uk/aboutus/events/>

School of Mathematics <http://www.mims.manchester.ac.uk/events/>

School of Physics and Astronomy <http://www.physics.manchester.ac.uk/aboutus/events/>

School of Mechanical, Aerospace and Civil Engineering <http://www.mace.manchester.ac.uk/>

School of Electrical and Electronic Engineering <http://www.eee.manchester.ac.uk/aboutus/news/>

School of Earth, Atmospheric and Environmental Sciences

<http://www.seaes.manchester.ac.uk/aboutus/events/>

Events

Application of Systems Approaches to Biologicals and their Production

Thursday 3rd November (10.00 – 16.30), MIB, University of Manchester, UK

The day will include Key note presentations on Expression systems and systems biology approaches with sessions on:

- Automation of cell based assays and production platforms
- Large data set generation associated with automation
- Progressing, integration and interpretation

MANCHESTER 1824

COEBP
Centre of Excellence in Biopharmaceuticals

mcfsb

Centre of Excellence in Biopharmaceuticals & Manchester Centre for Integrative Systems Biology Symposium

Application of Systems Approaches to Biologicals and their Production

THURSDAY 3RD NOVEMBER 2011 (10.00 – 16.30)
UNIVERSITY OF MANCHESTER, UK

Key note presentations:
- Expression systems and systems biology approaches

Sessions:
- Automation of cell based assays and production platforms
- Large data set generation associated with automation
- Progressing, integration and interpretation of multiple, large, data sets

Register at: www.coebp.is.manchester.ac.uk

EUROPEAN UNION
MANCHESTER
UNIVERSITY OF MANCHESTER

Northwest

of multiple, large, data sets.
To register please visit the [website](#)

Bruker UK SPM user meeting

Scanning Probe Microscopy Conference & User Meeting, University of Manchester, 22nd – 23rd November (held in the MIB)

- Presentations from leading academic and industry researchers
- Optimise your skills in Practical Workshops

The Bruker SPM Conference and Users Meeting will focus on exciting new SPM applications and recent technology developments. The meeting is open to anyone with an interest in characterisation at the nanoscale or Scanning Probe Microscopy and will act as an open forum for exchange of ideas. The main conference will take place from 9.30 to 16.00 on Wednesday November 23rd with topics including biomaterials interfaces, tribology, electrical characterisation, high resolution imaging, High-speed AFM studies and more. There will be a probes draw for delegates to win £1,000 of AFM probes.

Anybody wishing to register for this event or wanting to find out more should contact [Steve Marsden](#)



Bruker SPM Conference & Users' Meeting

Diet and the Gut Microflora in Health and Disease

Michael Smith Lecture Theatre, University of Manchester Friday 4th November 2011.

First Joint Meeting of the Diet, Digestion and Health Network and the European Network for Gastrointestinal Health Research. For further information contact: Nick Chadwick (n.chadwick@manchester.ac.uk)

Intensive 2-day workshop on NMR – 12th-13th January 2012

Following the success of the previous NMR workshops held in the January of 2010 and 2011, the next year's workshop is scheduled on 12th and 13th January 2012 in the School of Chemistry, University of Manchester. The on-line registration for this workshop is now open and full details can be found by following the web link below which includes a flyer to download. <http://www.chemistry.manchester.ac.uk/aboutus/events/nmr/>

Publications

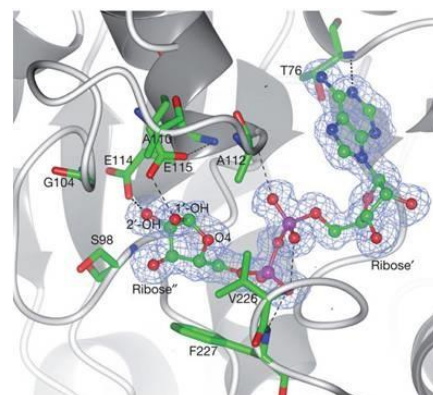
Publication Highlight

Bacteria shed light on new drug targets for inherited cancers

[The structure and catalytic mechanism of a poly\(ADP-ribose\) glycohydrolase.](#)

Slade D, Dunstan MS, Barkauskaite E, Weston R, Lafite P, Dixon N, Ahel M, Leys D, Ahel I. Nature. 2011 Sep 4. doi: 10.1038/nature10404. [Epub ahead of print]

Prof David Leys and colleagues at the University of Manchester's Paterson Institute for Cancer Research have succeeded in purifying a protein found in bacteria that could reveal new drug targets for inherited breast and ovarian cancers as well as other cancers linked to DNA repair faults. The team are the first to decipher the structure of a protein called PARG – which plays an important role in DNA repair and acts in the same pathway as PARP. PARP



inhibitors have been showing great promise in clinical trials for patients with breast, ovarian and prostate cancers caused by mutations in genes called BRCA1 and BRCA2. They work by blocking the action of PARP – a protein that chemically tags areas of DNA damage to highlight them to the cell's DNA repair machinery.

PARG removes these chemical tags after the DNA damage has been repaired. So the researchers believe that, similar to PARP inhibitors, drugs designed to block the action of PARG could be effective in treating cancer. Lead author Dr Ivan Ahel, based at the Cancer Research UK-funded Paterson Institute, said: "For decades scientists have wanted to find out the structure of PARG, but its large size makes it very hard to produce in the lab. By studying a smaller version of PARG found in bacteria, we've been able to create a '3D map' that researchers can use to understand more about how PARG works. The next step will be to investigate whether drugs that block its activity might be an effective way of treating cancers driven by faults in DNA repair genes." Co-author Professor David Leys, who is based in the Faculty of Life Sciences, said: "Obtaining the crystal structure of PARG is a first and key step to guide and illuminate future drug-design efforts aimed at treating certain cancers. Knowing what this enzyme looks like, and having a good idea of how it operates, makes designing such drugs less of a shot in the dark." Dr Julie Sharp, senior science information manager at Cancer Research UK, added: "This discovery shows that bacteria and humans share similarities in the cellular machinery they use to repair damaged DNA. Importantly, knowing the structure of PARG in bacteria could help researchers design targeted treatments that are also effective in cancer patients. We hope this will lead to further treatment options for patients with a range of cancers in the future."

Publications

Samrina Rehman, Royston Goodacre, Philip J Day, Ardeshir Bayat, Hans V Westerhoff Dupuytren's: a systems biology disease. *Arthritis Research & Therapy* 2011, **13**:238 (12 September 2011) [Paper](#)

Ioannou A, Cini E, Timofte RS, Flitsch SL, Turner NJ, Linclau B.

Heavily fluorinated carbohydrates as enzyme substrates: oxidation of tetrafluorinated galactose by galactose oxidase. *Chem Commun (Camb)*. 2011 Sep 13. [Epub ahead of print] [Paper](#)

Latifi R, Tahsini L, Kumar D, Sastry GN, Nam W, de Visser SP. Oxidative properties of a nonheme Ni(ii)(O(2)) complex: Reactivity patterns for C-H activation, aromatic hydroxylation and heteroatom oxidation. *Chem Commun (Camb)*. 2011 Sep 2. [Epub ahead of print] [Paper](#)

Geenen S, du Preez FB, Reed M, Frederik Nijhout H, Gerry Kenna J, Wilson ID, Westerhoff HV, Snoep JL. A mathematical modelling approach to assessing the reliability of biomarkers of glutathione metabolism. *Eur J Pharm Sci*. 2011 Aug 24. [Epub ahead of print] [Paper](#)

McCarty S, Syed F, Bayat A. Role of the HLA System in the Pathogenesis of Dupuytren's Disease. *Hand (N Y)*. 2010 Sep;5(3):241-50. Epub 2010 Feb 9. [Paper](#)

Liem SY, Shaik MS, Popelier PL. Aqueous Imidazole Solutions: A Structural Perspective from Simulations with High-Rank Electrostatic Multipole Moments. *J Phys Chem B*. 2011 Sep 9. [Epub ahead of print] [Paper](#)

Dunstan MS, Barnes J, Humphries M, Whitehead RC, Bryce RA, Leys D, Stratford IJ,

Nolan KA. Novel Inhibitors of NRH:Quinone Oxidoreductase 2 (NQO2): Crystal Structures, Biochemical Activity, and Intracellular Effects of Imidazoacridin-6-ones. *J Med Chem.* 2011 Sep 13. [Epub ahead of print] [Paper](#)

Griffin M, Iqbal SA, Sebastian A, Colthurst J, Bayat A. Degenerate Wave and Capacitive Coupling Increase Human MSC Invasion and Proliferation While Reducing Cytotoxicity in an In Vitro Wound Healing Model. *PLoS One.* 2011;6(8):e23404. Epub 2011 Aug 16. [Paper](#)

Sidgwick GP, Bayat A. Extracellular matrix molecules implicated in hypertrophic and keloid scarring. *J Eur Acad Dermatol Venereol.* 2011 Aug 12. doi: 10.1111/j.1468-3083.2011.04200.x. [Epub ahead of print] [Paper](#)

Wang X, McKendrick I, Barrett I, Dix I, French T, Tsujii J, Ananiadou S. Automatic Extraction of Angiogenesis Bio-Process from Text. *Bioinformatics.* 2011 Aug 5. [Epub ahead of print] [Paper](#)

Kell DB. Breeding crop plants with deep roots: their role in sustainable carbon, nutrient and water sequestration. *Ann Bot.* 2011 Sep;108(3):407-18. Epub 2011 Aug 3. [Paper](#)

Eyers CE, Lawless C, Wedge DC, Lau KW, Gaskell SJ, Hubbard SJ. CONSeQuence: prediction of reference peptides for absolute quantitative proteomics using consensus machine learning approaches. *Mol Cell Proteomics.* 2011 Aug 3. [Epub ahead of print] [Paper](#)

Ashcroft KJ, Syed F, Arscott G, Bayat A. Assessment of the influence of HLA class I and class II loci on the prevalence of keloid disease in Jamaican Afro-Caribbeans. *Tissue Antigens.* 2011 Aug 4. doi: 10.1111/j.1399-0039.2011.01755.x. [Epub ahead of print] [Paper](#)

Wedge DC, Allwood JW, Dunn W, Vaughan AA, Simpson K, Brown M, Priest L, Blackhall FH, Whetton AD, Dive C, Goodacre R. *Anal Chem.* Is Serum or Plasma More Appropriate for Intersubject Comparisons in Metabolomic Studies? An Assessment in Patients with Small-Cell Lung Cancer. 2011 Aug 2. [Epub ahead of print] [Paper](#)

Kinalwa M, Blanch EW, Doig AJ. Determination of protein fold class from Raman or Raman optical activity spectra using random forests. *Protein Sci.* 2011 Jul 15. doi: 10.1002/pro.695. [Epub ahead of print] [Paper](#)

Leferink NG, Pudney CR, Brenner S, Heyes DJ, Eady RR, Samar Hasnain S, Hay S, Rigby SE, Scrutton NS. Gating mechanisms for biological electron transfer: Integrating structure with biophysics reveals the nature of redox control in cytochrome P450 reductase and copper-dependent nitrite reductase. *FEBS Lett.* 2011 Jul 14. [Epub ahead of print] [Paper](#)

Heuts DP, Gummadova JO, Pang J, Rigby SE, Scrutton NS. Reaction of vascular adhesion protein-1 with primary amines: Mechanistic insights from isotope effects and quantitative structure-activity relationships. *J Biol Chem.* 2011 Jul 7. [Epub ahead of print] [Paper](#)

Please send comments and items for inclusion in the next newsletter to:
[Ros Le Feuvre](#) (Next edition deadline 10th Nov)